

Closing the pseudogap quietly.

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Abstract – The physical properties of hole-doped cuprate high-temperature superconductors are heavily influenced by an energy gap known as the pseudogap whose origin remains a mystery second only to that of superconductivity itself. A key question is whether the pseudogap closes at a temperature T^* . The absence of a specific heat anomaly, together with persistent entropy losses up to 300K, have long suggested that the pseudogap does not vanish at T^* . However, amid a growing body of evidence from other techniques pointing to the contrary we revisit this question. Here we investigate if, by adding a temperature dependence to the pseudogap energy and quasiparticle lifetime in the resonating-valence-bond spin-liquid model of Yang Rice and Zhang, we can close the pseudogap quietly in the specific heat.

The physical properties of hole-doped cuprate high-temperature superconductors are strongly influenced, over a wide range of temperature and doping, by a depletion in the electronic density of states known as the pseudogap. In momentum-space it is manifest as a gapping of the large hole-like Fermi surface near the antinodal regions of the Brillouin zone, at $(\pm\pi, 0)$ and $(0, \pm\pi)$, leaving behind ungapped “Fermi arcs” [1]. The origin of the pseudogap remains a mystery second only to that of high-temperature superconductivity itself, and it is widely hoped that by investigating the former we might uncover valuable insights for understanding the latter. A key question is whether the pseudogap closes at a temperature T^* . In recent years, evidence has been building that suggests that it does. These include abrupt changes in the Kerr Effect [2], time resolved reflectivity [3], as well as the direct observation of a reconstruction of the antinodal electronic structure by angle-resolved photoemission spectroscopy [3,4] (ARPES). In this work, we aim to reconcile those results with thermodynamic measurements, in particular the electronic entropy and specific heat, which have long suggested that the pseudogap is temperature independent [5–8].

By way of introduction, the electronic entropy is defined as $S(T) = -2k_B \int f_w(E, T) N(E) dE$ [9] where $N(E)$ is the density of states, and $f_w(E, T)$ is a “Fermi window” which expands with temperature and is related to the Fermi distribution function f by $f \ln f + (1-f) \ln(1-f)$. Put simply, $S(T)$ is a count of the thermally active states. The electronic specific heat coefficient is given by the temper-

ature derivative of the entropy, $\gamma(T) = \partial S(T) / \partial T$. Three apparently universal observations have been made from high-resolution differential specific heat studies on a variety of hole-doped cuprates [5–8, 10]. These are: i) a loss of entropy in low to slightly overdoped samples, that persists right up to the highest temperatures measured. The entropy decreases at a rate of about $1 k_B$ per doped hole; ii) a collapse in the magnitude of the specific heat jump, $\Delta\gamma$, at T_c below a critical doping of 0.19 holes/Cu; and iii) a smooth downturn in the normal-state electronic specific heat with no specific heat jump at T^* . These features were originally modeled by Loram in terms of a temperature-independent non-states-conserving V-shaped gap, pinned to the Fermi level (E_F) of a flat density of states. The gap widens with reducing doping [8]. In contrast to the superconducting gap, where the low-energy states are pushed just above the gap edge, it is surmised in this model that the pseudogap redistributes those states to much higher energies. In this scenario T^* represents an energy scale where thermal fluctuations become comparable in magnitude to the size of the pseudogap, rather than a phase transition temperature. If one tries to fill in such a pseudogap with temperature, thereby simulating expanding Fermi arcs [1, 11], problems arise. Firstly, the lost entropy is eventually recovered, contradicting (i). Secondly, a kink in the entropy appears at T^* together with a corresponding jump in the heat capacity [12], contradicting (iii). And finally, we might expect a double-peak structure to appear in the superconducting anomaly near

critical doping, where T^* is less than T_c , altering the doping dependence of $\Delta\gamma(T_c)$ compared to (ii). But perhaps this just means that this model is incomplete, and if so, what are we missing?

In the following we will investigate the effects of a tight-binding density of states, thermal lifetime broadening, and the combination of these with a Fermi-surface reconstruction model for the pseudogap given by the resonating valence bond spin liquid ansatz of Yang, Rice and Zhang (YRZ) [13]. Detailed descriptions of the YRZ model have been published several times [13–15], but for completeness we briefly list the equations used in this work. In the normal state the coherent part of the electron Green's function is given by

$$G(\mathbf{k}, \omega, x) = \frac{g_t(x)}{\omega - \xi_{\mathbf{k}} - \frac{E_g^2(\mathbf{k})}{\omega + \xi_{\mathbf{k}}^0}} \quad (1)$$

where $\xi_{\mathbf{k}} = -2t(x)(\cos k_x + \cos k_y) - 4t'(x) \cos k_x \cos k_y - 2t''(x)(\cos 2k_x + \cos 2k_y) - \mu_p(x)$ is the tight-binding energy-momentum dispersion, $\xi_{\mathbf{k}}^0 = -2t(x)(\cos k_x + \cos k_y)$ is the nearest-neighbour term, and $E_g(\mathbf{k}) = [E_g^0/2](\cos k_x - \cos k_y)$ is the pseudogap. The chemical potential $\mu_p(x)$ is chosen according to the Luttinger sum rule. The doping-dependent coefficients are given by $t(x) = g_t(x)t_0 + (3/8)g_s(x)J\chi$, $t'(x) = g_t(x)t'_0$ and $t''(x) = g_t(x)t''_0$, where $g_t(x) = 2x/(1+x)$ and $g_s(x) = 4/(1+x)^2$ are the Gutzwiller factors. The bare parameters $t'/t_0 = -0.3$, $t''/t_0 = 0.2$, $J/t_0 = 1/3$ and $\chi = 0.338$ are the same as used previously [13]. Equation 1 can be re-written as

$$G(\mathbf{k}, \omega, x) = \sum_{\alpha=\pm} \frac{g_t(x)W_{\mathbf{k}}^{\alpha}(x)}{\omega - E_{\mathbf{k}}^{\alpha}(x)} \quad (2)$$

where the energy-momentum dispersion is reconstructed by the pseudogap into upper and lower branches

$$E_{\mathbf{k}}^{\pm} = \frac{1}{2}(\xi_{\mathbf{k}} - \xi_{\mathbf{k}}^0) \pm \sqrt{\left(\frac{\xi_{\mathbf{k}} + \xi_{\mathbf{k}}^0}{2}\right)^2 + E_g^2(\mathbf{k})} \quad (3)$$

that are weighted by

$$W_{\mathbf{k}}^{\pm} = \frac{1}{2} \left[1 \pm \frac{(\xi_{\mathbf{k}} + \xi_{\mathbf{k}}^0)/2}{\sqrt{[(\xi_{\mathbf{k}} + \xi_{\mathbf{k}}^0)/2]^2 + E_g^2(\mathbf{k})}} \right] \quad (4)$$

In the superconducting state there are four energy branches $\pm E_S^{\alpha} = \pm \sqrt{(E_{\mathbf{k}}^{\alpha})^2 + \Delta_{\mathbf{k}}^2}$, where $\alpha = \pm$ and $\Delta_{\mathbf{k}} = [\Delta_0(x)/2](\cos k_x - \cos k_y)$ is the superconducting gap. The density of states (DOS), from which the entropy and heat capacity can be calculated, is given by

$$N(\omega) = \sum_{\alpha=\pm, \mathbf{k}} g_t(x)W_{\mathbf{k}}^{\alpha}[(u_{\mathbf{k}}^{\alpha})^2\delta(\omega - E_S^{\alpha}) + (v_{\mathbf{k}}^{\alpha})^2\delta(\omega + E_S^{\alpha})] \quad (5)$$

where $(u_{\mathbf{k}}^{\alpha})^2 = 0.5(1 + E_{\mathbf{k}}^{\alpha}/E_S^{\alpha})$ and $(v_{\mathbf{k}}^{\alpha})^2 = 0.5(1 - E_{\mathbf{k}}^{\alpha}/E_S^{\alpha})$ are the Bogoliubov weights.

The reason for choosing this model is because it successfully describes experimental data from a wide range of techniques [16], including the specific heat [17, 18]. However, the previous works did not consider a temperature dependent pseudogap term. In fig. 1 we plot the calculated energy momentum dispersion in the superconducting state along cuts in the k_y direction near the antinodes for $x=0.12$, both with, and without ($E_g=0$) the pseudogap. The results reproduce the ARPES-derived dispersions measured below and above T^* respectively [3, 4], providing compelling evidence for the closure of the pseudogap at T^* . Key details are reproduced such as the separation between the momentum of the minimum binding energy of the dispersion k_G from the Fermi momentum k_F , a signature of non-particle-hole symmetric order [4]. Moreover we can identify the flat dispersion of the shoulder feature observed in ARPES energy dispersion curves [3] as belonging to the Bogoliubov dispersion arising from the upper YRZ band, $-\sqrt{(E_{\mathbf{k}}^+)^2 + \Delta_{\mathbf{k}}^2}$.

Since we wish to understand the effect of adding a temperature dependence to E_g , from here onwards we fix the tight binding coefficients to their values at $x=0.20$ and neglect the $g_t(x)$ prefactor in the equation for the density of states. (Normally the x dependence of these terms, which narrow the bands but reduce the magnitude of the DOS, would complement rather than counteract the pseudogap.) To fit the experimental entropy data t_0 is set to 0.225 eV. Beginning for a moment without the pseudogap, the defining feature of the tight-binding DOS is the van Hove singularity (vHs) located just below E_F for $x=0.20$ (see fig. 2(a)). Assuming a rigid shift of E_F away from the vHs with decreasing doping results in a persistent decrease in entropy, as shown in fig. 2(d). However at 300 K, the rate of decrease is only 0.33 k_B /hole compared with the observed 1 k_B /hole [8].

Lifetime broadening can also affect the high-temperature heat capacity, and hence the entropy, by smoothing features in the DOS [19]. From resistivity measurements [20] we infer a linear-in-temperature scattering rate (inverse lifetime) given by $\Gamma = 0.01t_0 + \beta k_B T$, with a slope β that increases with decreasing doping. The most computationally efficient way of incorporating this term is by convolving the DOS with the lorentzian $\Gamma/\pi[(\omega - E)^2 + \Gamma^2]$. Figure 2(b) illustrates the thermally broadened vHs at 300 K for $x=0.20$ and 0.14 with $\beta=1$ and 2 respectively. The entropy decrease is now larger at 0.7 k_B /hole (fig. 2(e)), but it is still not enough, especially at low temperatures. This necessitates the incorporation of a pseudogap.

In fig. 2(c) we add a pseudogap for $x=0.14$ by setting $E_g^0=54$ meV. Based on the ARPES results we initially assume that the pseudogap closes linearly with temperature according to $E_g(T) = E_g^0 - 2k_B T$. The van Hove singularity and lifetime broadening effects are also included. The calculated entropy compares well with experimental data for $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ [6], shown in fig. 2(f), with the en-

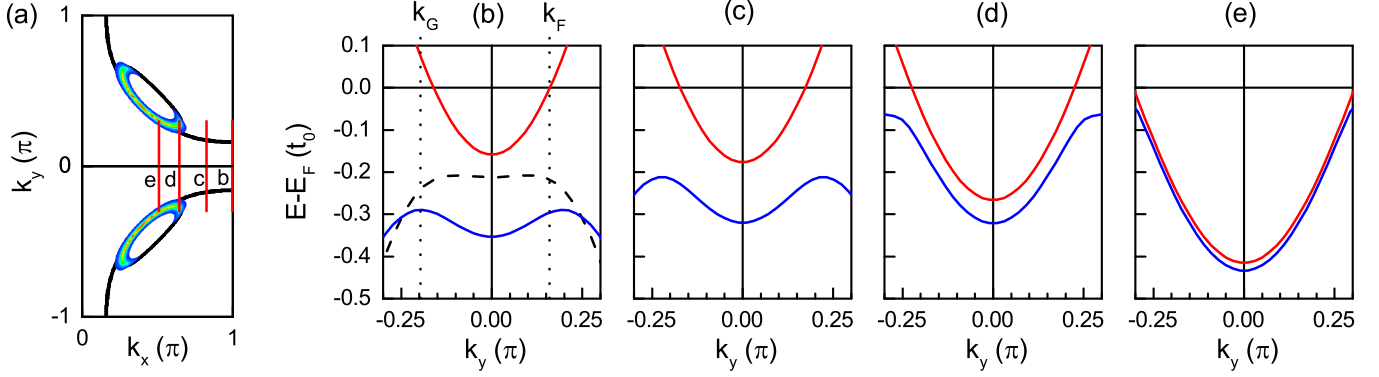


Fig. 1: (Color online) (a) Spectral weight at the Fermi level calculated from the YRZ model for $x=0.12$. The black curves indicate the back of the nodal hole pocket, as well as the Fermi level crossings when $E_g=0$. Dispersions calculated along the vertical momentum-space cuts are shown in plots (b) to (e), both with (blue line) and without (red line) the pseudogap. In the $k_x = \pi$ cut, (b), the dashed line shows the Bogoliubov dispersion from the upper YRZ band ($\Delta_0=0.12t_0$). These results closely reproduce the experimental data of Refs. [4] and [3]

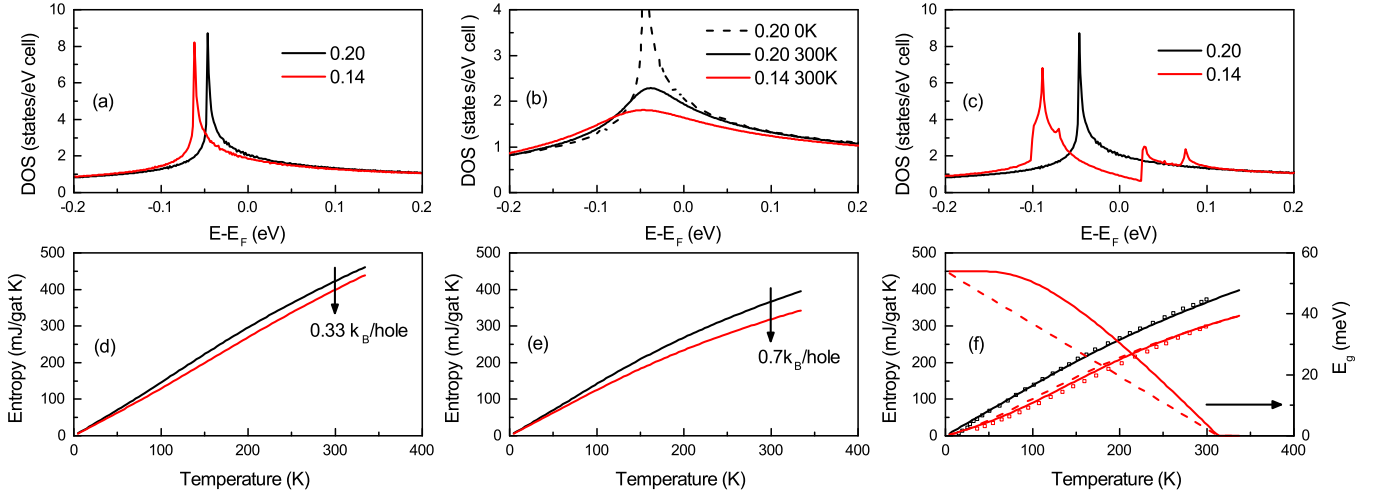


Fig. 2: (Color online) Density of states for $x=0.20$ and 0.14 in the case of: (a) a rigid shift of the Fermi level and no lifetime broadening; (b) the addition of thermal lifetime broadening terms $\pi k_B T$ and $2\pi k_B T$ respectively; and (c) a YRZ-like reconstruction. The corresponding electronic entropies are shown in plots (d) to (f). Plot (f) includes experimental data for $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ [6] and the calculated curves include the thermal broadening terms. The two fits to the $x=0.14$ data correspond to the two pseudogap temperature dependences of $E_g(T)$.

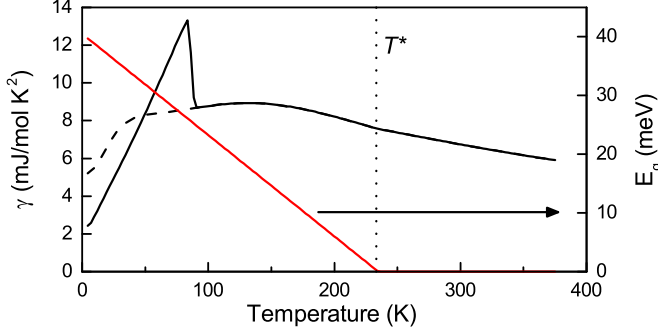


Fig. 3: (Color online) Electronic specific heat for a YRZ-like pseudogap that closes as $E_g = E_g^0 - 2k_B T$ in the presence of lifetime broadening $\Gamma = 0.01t_0 + k_B T$. Note the absence of a specific heat jump at T^* .

entropy decrease approaching the observed $1 k_B$ /hole. The low-temperature fit can be further improved by taking a more gradual initial T -dependence given by

$$E_g(T) = E_g^0 \left[2 - 1 / \tanh \left(\frac{E_g^0 \ln 3}{4k_B T} \right) \right] \quad (6)$$

We now turn to the specific heat coefficient, γ . Figure 3 shows $\gamma(T)$ calculated for a 40meV pseudogap which closes linearly with temperature in the presence of lifetime broadening with $\beta=1$. (This of course does not contain the additional experimentally observed contributions from fluctuations near T_c .) There is no obvious jump at T^* , only a slight change in slope. If $E_g(T)$ was rounded near T^* , due to doping inhomogeneity for example, the specific heat would become even smoother there. Finally, in fig. 4 we plot the doping dependence of the specific heat jump at T_c assuming a parabolic superconducting gap doping dependence $\Delta(x) = 0.103t_0[1 - 82.6(x - 0.16)^2]$, and the YRZ pseudogap doping dependence $E_g^0(x) = 3t_0(0.2 - x)$ for $x \leq 0.2$. Here we take the closure of the pseudogap to lie at $x = 0.2$ in continuity with YRZ, however it has been extensively shown that this occurs at slightly lower doping $x = 0.19$ [21]. The pseudogap model reproduces the collapse of the specific heat jump as reported for example in refs. [10] and [8]. Note that here we have taken a doping independent lifetime broadening, $\beta = 1$. Increasing β with decreasing doping would increase the rate of collapse of $\Delta\gamma(T_c)$.

To conclude, the absence of a specific heat jump at T^* , together with persistent losses in entropy at high temperatures, has long been taken as evidence that the pseudogap does not close there. Driven by a growing body of evidence from other experimental probes pointing to the contrary we have explored this question. By adding a linear-in-temperature scattering rate to a YRZ-like reconstruction model, it is possible to close the pseudogap quietly in the specific heat. A similar result is expected for the antiferromagnetic Brillouin-zone-folding Fermi surface reconstruction model [22]. The entropy recovery expected from the

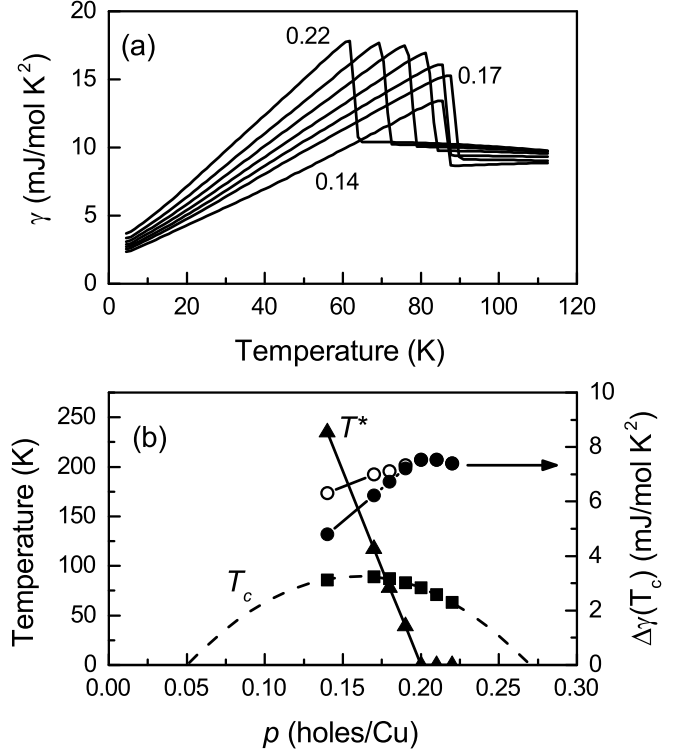


Fig. 4: (a) Superconducting electronic specific heat jump for $x=0.14$, and 0.17 to 0.22 , in the presence of a YRZ-like pseudogap that closes as $E_g = E_g^0 - 2k_B T$ and lifetime broadening $\Gamma = 0.01t_0 + k_B T$. (b) Doping dependence of T_c (squares), T^* (triangles), and the specific heat jump at T_c both with (filled circles) and without (empty circles) the pseudogap.

closing gap is offset by scattering-induced broadening of the van Hove singularity. This scenario could be tested experimentally by searching for an ongoing divergence between neighbouring entropy curves above T^* .

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